

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) er024_sq

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: er024_sq

Bond precision:	C-C = 0.0058 A	Wavelength=0.71073
Cell:	a=15.6794(4)	b=13.2596(4) c=19.9294(6)
	alpha=90	beta=104.551(3) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	4010.5(2)	4010.5(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C36 H16 Li O12 Zn2 [+ solvent]	?
Sum formula	C36 H16 Li O12 Zn2 [+ solvent]	C40 H29 Li N2 O12 Zn2
Mr	778.21	867.33
Dx, g cm ⁻³	1.289	1.436
Z	4	4
Mu (mm ⁻¹)	1.250	1.260
F000	1564.0	1768.0
F000'	1567.03	
h,k,lmax	21,18,27	19,16,26
Nref	5257	4510
Tmin,Tmax	0.746,0.893	0.951,1.000
Tmin'	0.662	

Correction method= # Reported T Limits: Tmin=0.951 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.858 Theta(max)= 28.881

R(reflections)= 0.0493(4127) wR2(reflections)= 0.1383(4510)

S = 1.087 Npar= 249

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT213_ALERT_2_C	Atom C105	has ADP max/min Ratio	3.1	prolat
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	3	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		4	Check

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C40 H29 Li1 N2 O12 Zn2

Atom count from the _atom_site data: C36 H16 Li1 O12 Zn2

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum C40 H29 Li N2 O12 Zn2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	160.00	144.00	16.00
H	116.00	64.00	52.00
Li	4.00	4.00	0.00
N	8.00	0.00	8.00
O	48.00	48.00	0.00
Zn	8.00	8.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	16	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	22.95	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C203 --C204 .	11.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C207 --C208 .	11.3	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of C204 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C205 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C206 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C207 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H204 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H205 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H206 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H207 Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	8%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C202 -C208_h .	1.46	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C203 -C208 .	1.46	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C203 -C208	0.16	Ang.
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	208	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	2.05	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	106	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	640	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.3	Low
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units

PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	2 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	2 Units
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
39 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
5 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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